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# Status of Structural Analysis of Substrates and Film Growth Inputs for GaN Device Development Program

**by Kevin Kirchner**

**ARL-TR-5427** **January 2011**

## NOTICES

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# Status of Structural Analysis of Substrates and Film Growth Inputs for GaN Device Development Program


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**Sensors and Electron Devices Directorate, ARL**

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**14. ABSTRACT**

This report covers the x-ray diffraction crystallographic analysis of semiconductor wafers involved in our team's project to produce gallium nitride (GaN) wide bandgap devices. The wafers were examined for crystal quality by symmetric and asymmetric GaN scans for each quadrant of the 18 wafers. Data comparisons made include the figures of merit (FOM) for GaN substrates compared with those of GaN films grown on the substrates, and the homoepitaxial GaN films' FOMs compared with those from heteroepitaxial films. The analysis produced the best FOMs for GaN for our lab to date: 39" (arc seconds) symmetric and 58" asymmetric. The good homoepitaxial GaN film quality was ~3 to 8 times better than that of good heteroepitaxial films. The heteroepitaxial GaN film quality was shown to be suited for our experimental needs. At a 95% confidence level, we were able to show a bias between the quality of the wafer quadrants of the Hydride Vapor Phase epitaxially grown GaN substrates. The microstructural quality of the material inputs as measured by x-ray diffraction is currently on track to play its part in the development of novel GaN-based devices.

**15. SUBJECT TERMS**

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## Acknowledgments

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# 1. Introduction and Background

Solid-state devices based on gallium nitride (GaN) have the potential to have superior electronic properties. After the type of material used, the quality of that material is critical. However growing and processing better materials is a laborious and very expensive process. An extremely useful way of tracking the material improvement process is through the use of x-ray diffraction. The wavelengths of the x-rays used are dimensionally on the scale of the smallest component (unit cell) of the atom's long range order. It is because of this relationship that x-ray diffraction is able to tell us how repeatable a group of unit cells are with respect to their neighbors. The higher the degree of repeatability in a crystalline solid, the higher the quality. The x-ray diffraction unit of measure of a material's quality is the full width at half maximum (FWHM) value.

This report covers the crystallographic analysis, by x-ray diffraction, of 18 recent wafers involved in our team's project to produce GaN-based wide bandgap (WBG) devices. The substrate and film inputs for the project came from Kyma, Crystal Systems, Mike Derenge, and our State University of New York (SUNY) partners. Some additional enabling collaborations during this period were with Georgia Institute of Technology, Pennsylvania State University, and Sandia National Laboratory. The wafers were examined by symmetric (sym) GaN (002) and asymmetric (asym) GaN (102) scans for each of the sub regions of the 18 wafers.

Besides the analysis of the basic crystalline quality of the project's inputs, many comparisons were made. For example, the figures of merit (FOMs) for GaN substrates were compared with the FOMs of GaN films that were grown on those substrates. Some comparisons between different FOMs are given in terms of percentage of improvements. So for example, if sample A had a FWHM value of 100" (arc seconds) and sample B had a FWHM value of 60", that comparison could be expressed as there being a 40% improvement between sample A and B. Also, it is worth noting that smaller FWHM values indicate better crystalline quality of a material.

Heteroepitaxially grown GaN films are still, relatively speaking, immature; and homoepitaxial GaN films, and the GaN substrates that make their existence possible, have even shorter analysis baselines. Because of the small number of good GaN homoepitaxial films currently available to us, this report is somewhat interim in nature. That said, my work has uncovered many encouraging material attributes. For example, the x-ray work includes the best FWHM numbers that I have measured for the GaN (002) peak, 39". FWHM values correlate with lower defect densities, and lower defect densities have been shown to correlate with better device characteristics.

With new material systems there are always challenges. The asymmetric x-ray scans seem to have revealed in plane, material quality issues. Many of these problems are conjectured to be caused by small angle grain boundaries (SAGBs).* SAGBs are thought to be formed by an amassing of line defects.

This work, besides documenting the overall quality of the material, also differentiates between multiple technologies, different material processing, and interactions between inputs. Additionally this work constitutes an initial investment in being able to make "before and after" comparisons in the future.

At this stage of the project, I am not sure of what and how patterns in the data will show up, so I employ a number of different methods of organizing the data in this report, i.e., graphical, chart form, grouping levels, and overlays. Each section of the report includes a short section-specific introduction.

This report contains six sections:

1. Introduction and Background
2. Kyma GaN substrates
3. SUNY heteroepitaxial GaN films
4. GaN substrates and film comparisons
5. Homoepitaxial vs. heteroepitaxial GaN films
6. Observations and Conclusions

*Callister, W. D. *Material Science and Engineering An Introduction*, Fourth Edition, John Wiley & Sons: New York 1997, p.77.

## 2. Kyma GaN Substrates

Twelve of Kyma's novel hydride vapor phase epitaxy (HVPE) GaN substrates, enabling homoepitaxial growth of GaN films, were analyzed. For analytical purposes, the twelve 1x1 cm wafers were divided into a total of 48 quadrants (Cartesian coordinate nomenclature). Each plot and major chart entry is labeled with the sample number from which it came. The plot's abscissa values are the quadrant number from which the data was taken; the ordinates are the FWHM values.

Notes:

- The plots of the x-ray scans were grouped by similarities of pattern. Patterns varied from having both sym (GaN 002) and asym (GaN 102) scans matching their counterparts to only having one of the pairs possess some similarity. There were also a couple of mirror image pairings between scans.
- The sym scans contained the best GaN FWHM value (39") I have seen to date. The asym values ranged from decent to poor. Sample 15691 (figure 1) had the best symmetric scans, averaging 40" across the four quadrants of its wafer. Quadrant I, for both sym and asym scans, had the best results across all samples. This could be caused by an inhomogeneity in the wafer's growth conditions. If an examination of the growth conditions turned up a difference it could potentially mean a significant improvement in the quality of the sample output as a whole. To be sure, we ran a statistical analysis and there is a statistically significant bias between the wafer quarters across the wafers (see the appendix). A level of detail of the scans that is not made clear by either the charts or the plots is the effect of an amassing of material defects, which create what are called SAGBs (figure 2).

## Ranking of Kyma's GaN Substrates by X-ray Diffraction

Kyma Substrates, Symmetric Scan (002), Units: Arc Seconds

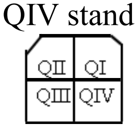
| | Wafer # | QI* | QII | QIII | QIV | Row Ave | Wafer Rank |
|---|---|---|---|---|---|---|---|
| | 6921 | 82 | 84 | 173 | 114 | 113 | 10 |
| | 6942 | 56 | 61 | 54 | 54 | 56 | 2 |
| | 7041 | 56 | 69 | 93 | 82 | 75 | 5 |
| | 7286 | 76 | 119 | 130 | 69 | 99 | 8 |
| | 8183 | 49 | 83 | 65 | 54 | 63 | 4 |
| | 8184 | 74 | 70 | 132 | 69 | 86 | 6 |
| | 8185 | 167 | 154 | 157 | 154 | 158 | 11 |
| | 8186 | 58 | 60 | 66 | 57 | 60 | Tie 3 |
| | 8187 | 72 | 157 | 85 | 72 | 97 | 7 |
| | 12932 | 100 | 101 | 104 | 120 | 106 | 9 |
| | 15691 | 39 | 39 | 40 | 41 | 39.75 | Best 1 |
| | 15994 | 54 | 60 | 61 | 65 | 60 | Tie 3 |
| **Averages** | | 74 | 88 | 97 | 79 | | |
| **Quad Ranking** | | 1st (Best) | 3rd | 4th | 2nd | | |

Kyma Substrates, Asymmetric Scan (102), Units: Arc Seconds

| | Wafer # | QI | QII | QIII | QIV | Row Ave | Wafer Rank |
|---|---|---|---|---|---|---|---|
| | 6921 | 525+204 | 402+342 | 551+321 | 624+164 | 858 | 5 |
| | 6942 | 700 | 1033 | 995 | 993 | 930 | 6 |
| | 7041 | 830 | 1225 | 1279 | 843 | 1044 | 8 |
| | 7286 | 823 | 1172 | 1344 | 962 | 1075 | 9 |
| | 8183 | 414 | 484 | 426 | 402 | 431 | 2 |
| | 8184 | 477 | 564 | 670 | 545 | 564 | 3 |
| | 8185 | 356 | 372 | 355 | 364 | 361 | Best 1 |
| | 8186 | 967 | 1217 | 1202 | 946 | 1083 | 10 |
| | 8187 | 1008 | 1385 | 1263 | 937 | 1149 | 11 |
| | 12932 | 1094 | 1756 | 1727 | 1172 | 1437 | 12 |
| | 15691 | 544 | 648 | 656 | 542 | 598 | 4 |
| | 15994 | 930 | 1161 | 1123 | 881 | 1024 | 7 |
| **Averages** | | 739 | 980 | 993 | 781 | | |
| **Quad Ranking** | | 1st (Best) | 3rd | 4th | 2nd | | |

Figure 1. Ranking of Kyma's GaN substrates by x-ray diffraction.

In figure 1, the following apply:

- QI through QIV stand for the different wafer quadrants. They are in Cartesian coordinates as follows: 


- There are 96 data points over 48 sample regions across 12 wafers.
- The asymmetric rocking curves (RCs) of sample 692.1 consisted of two distinct regions. The FWHM for each are included.

- For row and column averages, it is the sum of the two values that are used for sample 692.1.
- The row averages are also the sample average.

In addition to the rankings shown in the charts, the following was observed:

- The sym scans show a remarkable improvement over the industry standard.
- Up to their point in the sample stream, samples 8183, 8184, and 8185 were the 2nd, 3rd, and 1st, respectively, in in-plane (parallel to surface to sample) crystal quality. With sample 8186, the quality changed abruptly. Interestingly, the rankings of the quadrants across all samples are the same for both the sym and asym scans.

Figure 2 shows four scans (A through D). Scans A and B, although having similar FWHM numbers, show the start of a move from a monolithic to a multifaceted “flat topped” peak. With their flat-topped multifaceted peaks, scans C and D show the progression of the effect due to a further increase in the density of the SAGB.

Figure 3 presents a thumbnail overview of the GaN substrate plots.

Figures 4–6 show the enlarged individual plots.

The data from these x-ray scans of freestanding GaN substrates provides the first sets of data that allow subsequent comparisons between substrates and films and a more complete analysis between homoepitaxial and heteroepitaxial film growth. Eventually, the information will be carried forward into the analysis space where the processing and performance of devices is analyzed.

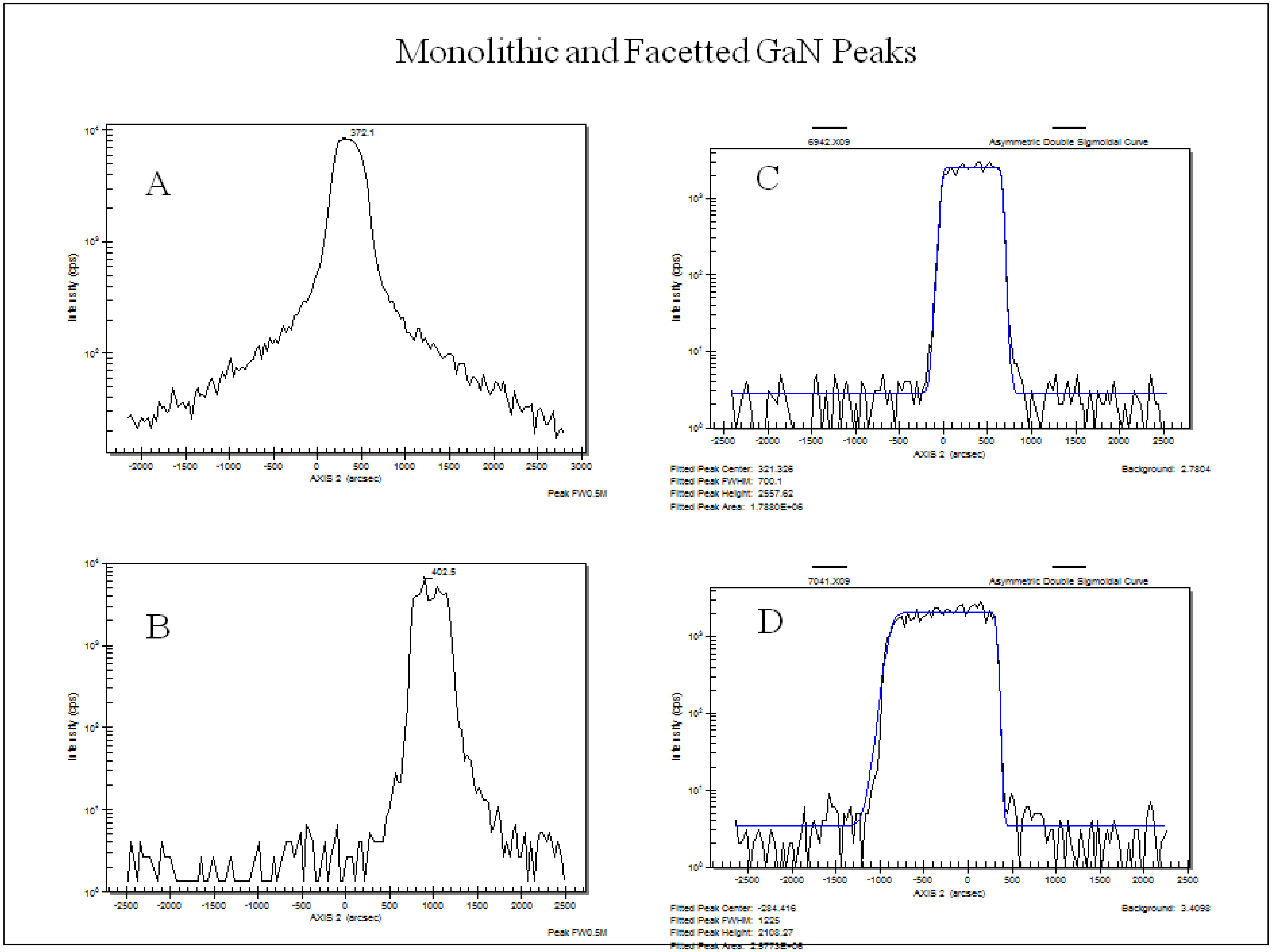
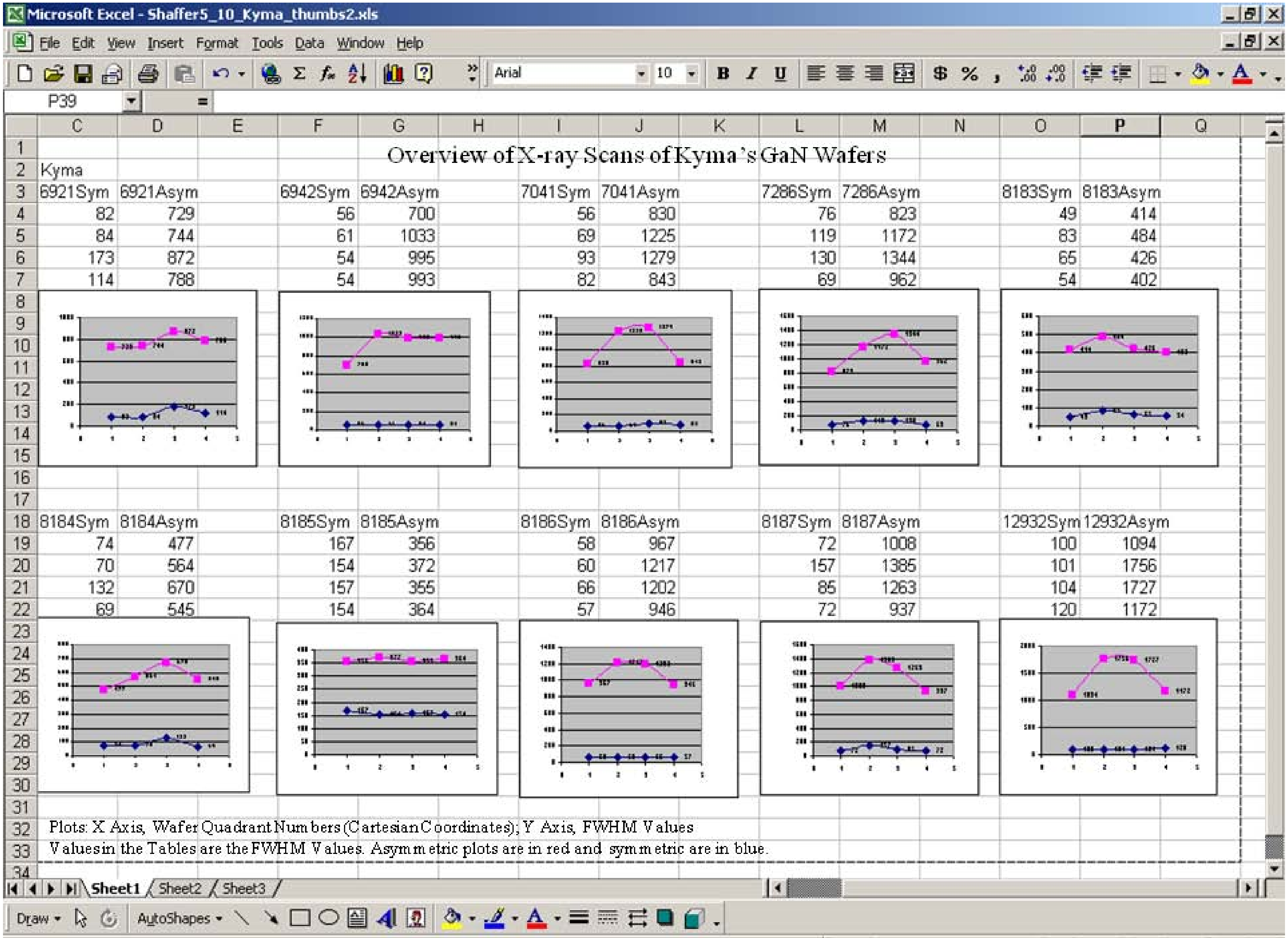



Figure 2. Scans of the monolithic and facetted GaN peaks. The plots are of intensity vs. position.



Overview of X-ray Scans of Kyma's GaN Wafers

Kyma

| 6921Sym | 6921Asym | 6942Sym | 6942Asym | 7041Sym | 7041Asym | 7286Sym | 7286Asym | 8183Sym | 8183Asym |
|---|---|---|---|---|---|---|---|---|---|
| 82 | 729 | 56 | 700 | 56 | 830 | 76 | 823 | 49 | 414 |
| 84 | 744 | 61 | 1033 | 69 | 1225 | 119 | 1172 | 83 | 484 |
| 173 | 872 | 54 | 995 | 93 | 1279 | 130 | 1344 | 65 | 426 |
| 114 | 788 | 54 | 993 | 82 | 843 | 69 | 962 | 54 | 402 |

| 8184Sym | 8184Asym | 8185Sym | 8185Asym | 8186Sym | 8186Asym | 8187Sym | 8187Asym | 12932Sym | 12932Asym |
|---|---|---|---|---|---|---|---|---|---|
| 74 | 477 | 167 | 356 | 58 | 967 | 72 | 1008 | 100 | 1094 |
| 70 | 564 | 154 | 372 | 60 | 1217 | 157 | 1385 | 101 | 1756 |
| 132 | 670 | 157 | 355 | 66 | 1202 | 85 | 1263 | 104 | 1727 |
| 69 | 545 | 154 | 364 | 57 | 946 | 72 | 937 | 120 | 1172 |

Plots: X Axis, Wafer Quadrant Numbers (Cartesian Coordinates); Y Axis, FWHM Values

Values in the Tables are the FWHM Values. Asymmetric plots are in red and symmetric are in blue.

Figure 3. Overview of the x-ray scans of Kyma's GaN wafers.

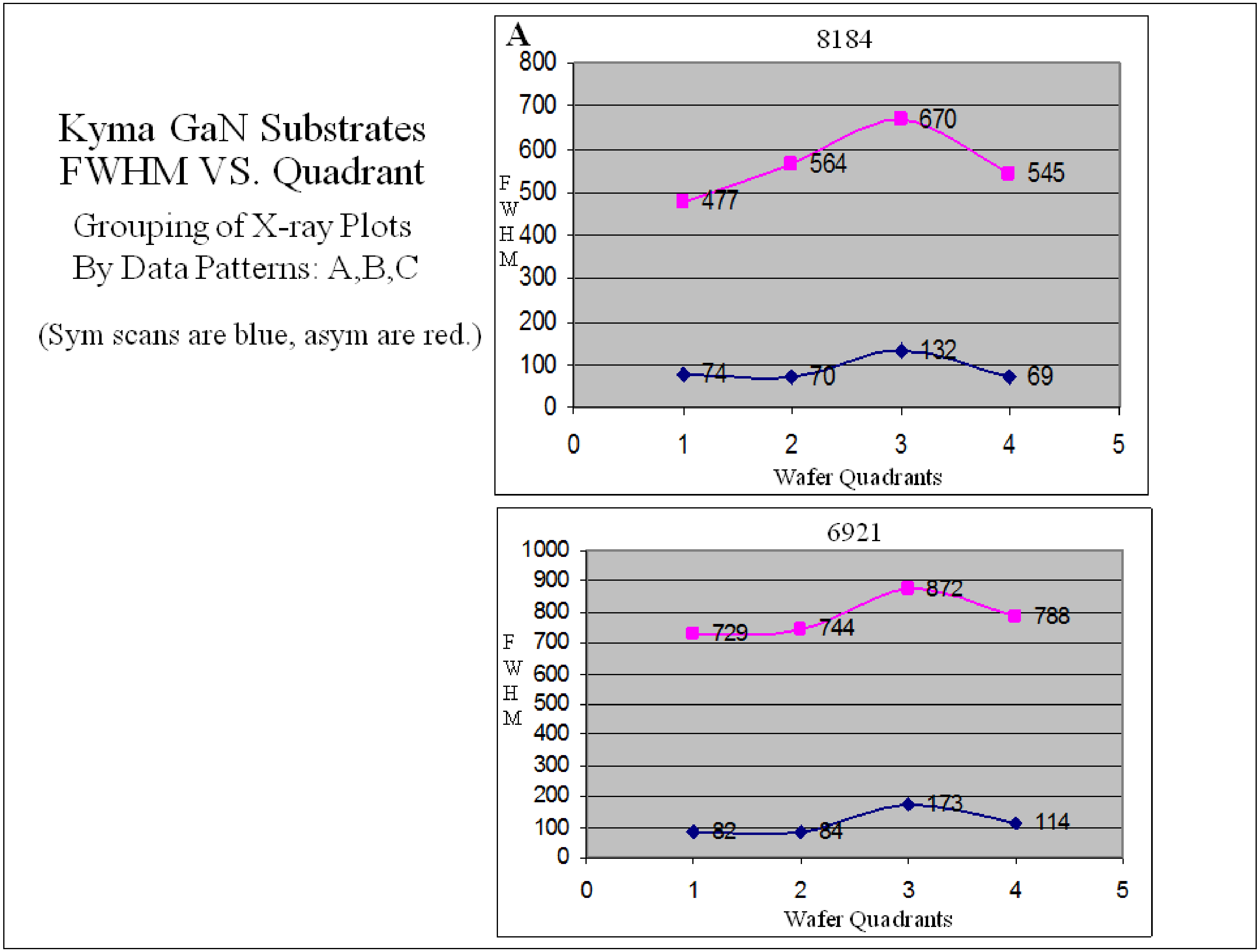



Figure 4. Kyma GaN substrates, FWHM vs. quadrant plots. The grouping shows data pattern A.

Note: The sym scans are blue and the asym scans are red.

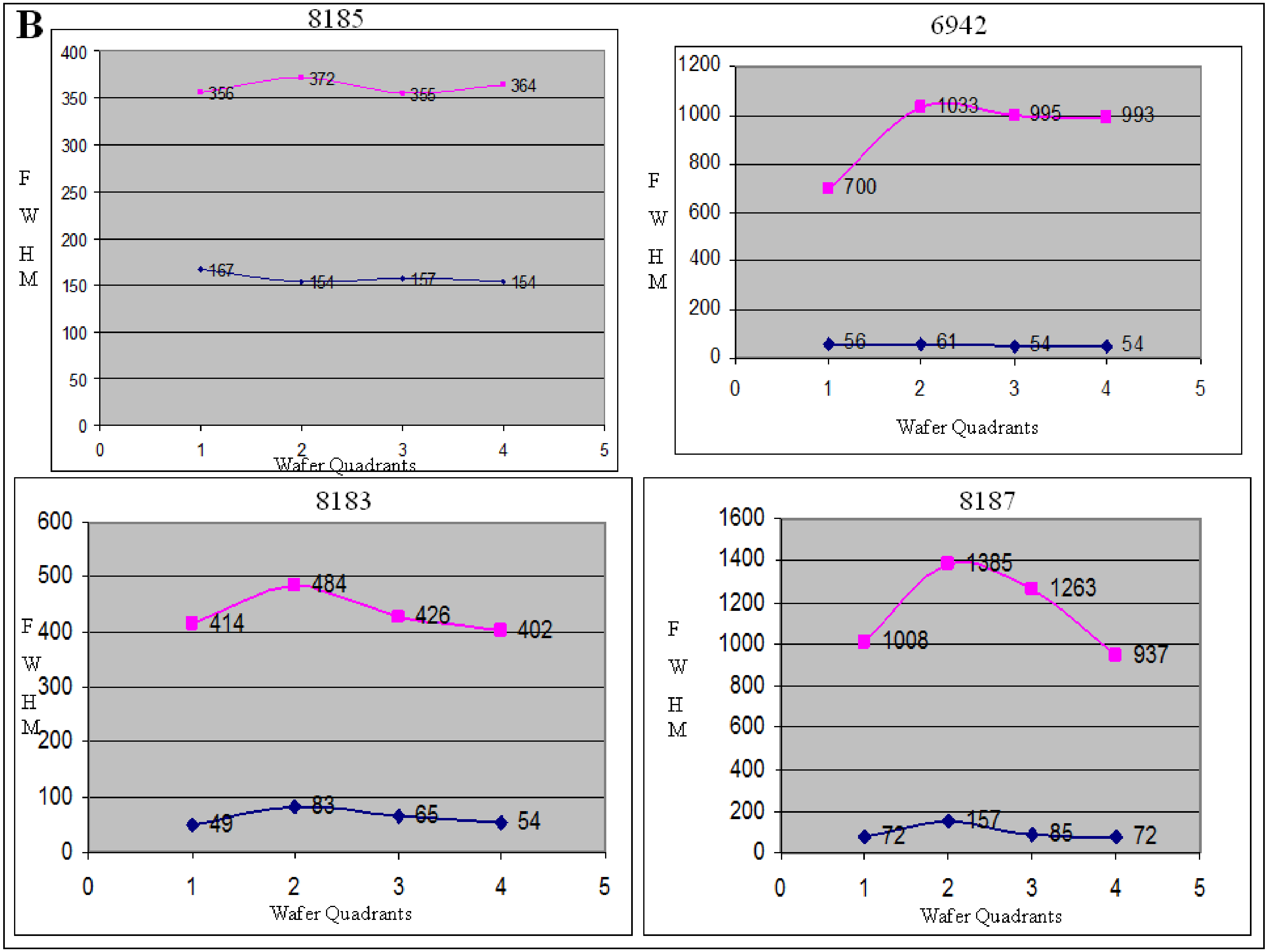



Figure 5. Kyma GaN substrates plots, FWHM vs. quadrant. The grouping of the plots shows data pattern B. Sym scans are blue and asym are red.

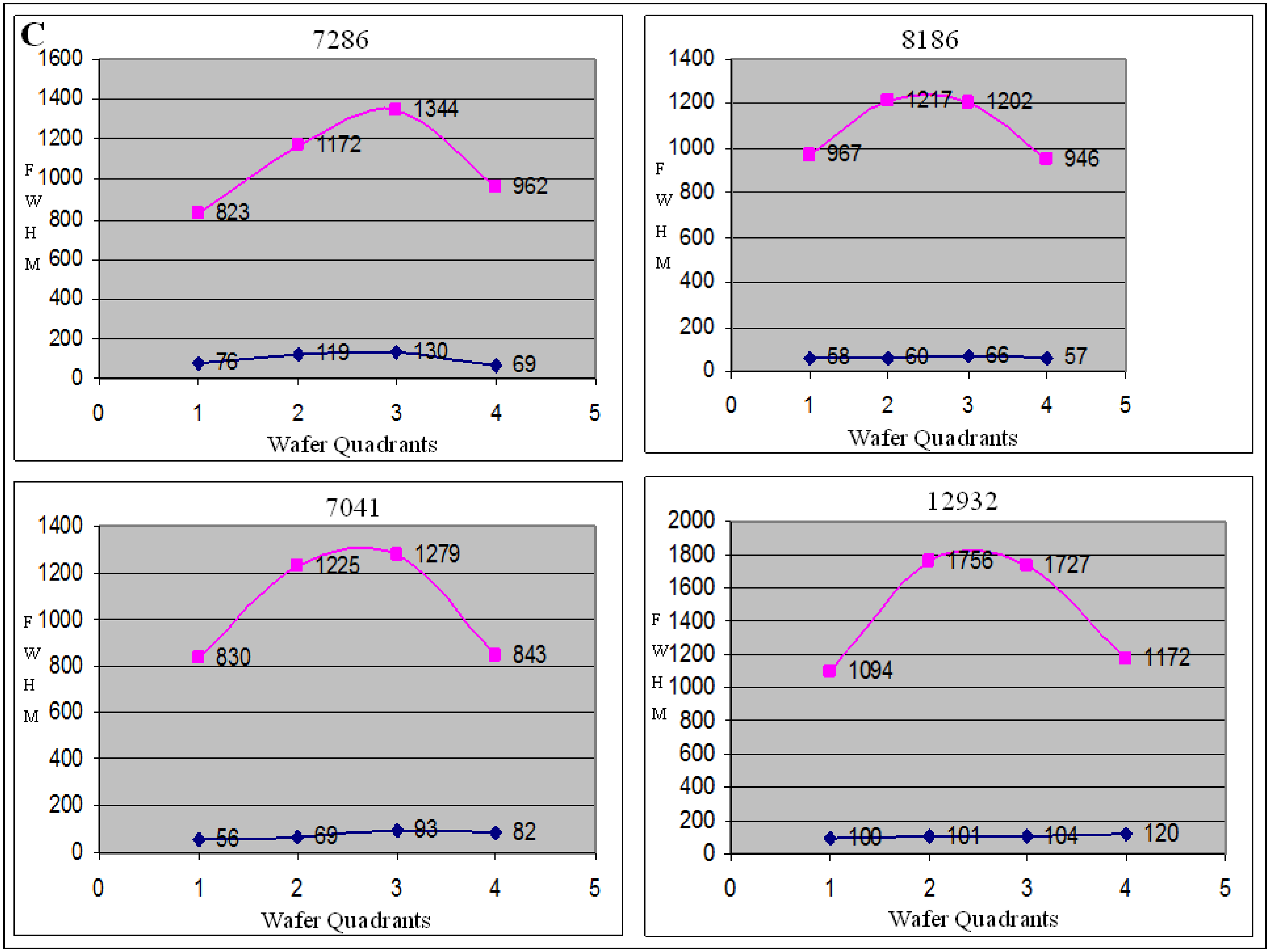



Figure 6. Kyma GaN substrates, FWHM vs. quadrant plots. The grouping of x-ray plots shows data pattern C.

Note: The sym scans are blue and the asym scans are red.

# 3. SUNY Heteroepitaxial GaN Films on Sapphire Substrates

Sym and asym scans were taken of the heteroepitaxial GaN films that were grown on five 2” sapphire wafers by our partners at SUNY. There is one x-ray plot per wafer containing both sym and asym scans (figure 8). Groupings of x-ray scans were again made on the basis of plot similarities (figure 9 and 10). Sample 2093N1 is one-half of a 2” wafer, having Quads I and IV. The collected data is also presented in chart form (figure 7). The chart shows rankings of the wafers and the quadrants across all SUNY wafers. The best wafer in terms of sym x-ray scans is 2093N. There was a tie for the best sample in terms of the asym scans, between samples 2079 and 2088. The best quadrant across all the wafers, in sym terms is QII. The best in terms of the asym scan analysis across all wafers is QI.

Note: Samples 2080 and 2088 were grown to be high electron mobility transistors (HEMTs) structures while the remaining samples were prepared to be Schottky devices. This means that the GaN films on 2080 and 2088 are thinner than those on the remaining samples. In heteroepitaxial growth, thicker films often show better structural quality than thinner films. Therefore if the two HEMT samples have similar or slightly worst FOMs this still signifies films of good quality in my opinion. Overall, sample 2080 had the second best scan out of the five samples for both sym and asym scans, and sample 2088 was the third best for sym scans and was tied for first for asym scans. Therefore, the HEMT samples echo the Schottky data, i.e., all our SUNY samples are of good microstructural quality.

These x-ray scans of the heteroepitaxial films are part of my group’s analysis and documentation of the input streams for our GaN Device Program. In this report additional analyses are presented, for example, I compare the Kyma homoepitaxial films with these heteroepitaxial films in section 4. Over time, as we learned the quality of the samples and our expectations for the project grew, we increased the number of scans from 8 scans per 2” sample to 32. Our team has been developing GaN Schottky diodes and HEMTs with segments of these wafers.

SUNY

Ranking of GaN / Sapphire Samples Using X-ray Diffraction

| Wafer # | | QI* | QII | QIII | QIV | Averages Sym | Averages Asym | Wafer Rank Sym | Wafer Rank Asym | Notes |
|---|---|---|---|---|---|---|---|---|---|---|
| 2079 | Sym | 313 | 302 | 335 | 342 | 323 | | 4 | | 8 data pts (dps), 4 & 4 |
| | Asym | 413 | 434 | 459 | 459 | | 441 | | 1a | |
| 2080 | Sym | 266 | 250 | 269 | 277 | 266 | | 2 | | |
| | Asym | 411 | 432 | 472 | 462 | | 444 | | 2 | 8 dps, 4 &4 |
| 2088 | Sym | 271 | 254 | 274 | 288 | 272 | | 3 | | 32 dps |
| | Asym | 403 | 404 | 481 | 474 | | 441 | | 1b | |
| 2093N | Sym | 230 | 222 | 230 | 243 | 231 | | 1 | | 32 dps |
| | Asym | 437 | 453 | 459 | 450 | | 450 | | 3 | |
| 2093N1 | Sym | 227 | | | 237 | 232 | | | | 1/2 wafer, 16 data pts |
| | Asym | 425 | | | 416 | | 421 | | | 16 dps, 8&8 |
| Averages | Sym | 261 | 206 | 222 | 277 | | | | | |
| | Asym | 418 | 431 | 468 | 452 | | | | | |
| Quad Rank | Sym | 3 | 1 | 2 | 4 | | | | | |
| | Asm | 1 | 2 | 4 | 3 | | | | | |

Notes

* QI - QIV stands for quadrants, using Cartesian coordinates

Table units are arc seconds

Symmetric scan values were in the good to excellent range

Asymmetric peaks also showed v. good FOM, had a narrow range, and the peaks were monolitic

Different sampling strategies over time made for inefficient use of data

Top half of wafers were slightly better than the bottom half.

Left side of samples ~ 25% better than right half for sym scans. Very close for asym peaks, slight advantage R side

Figure 7. Ranking of SUNY GaN/sapphire samples using x-ray diffraction.

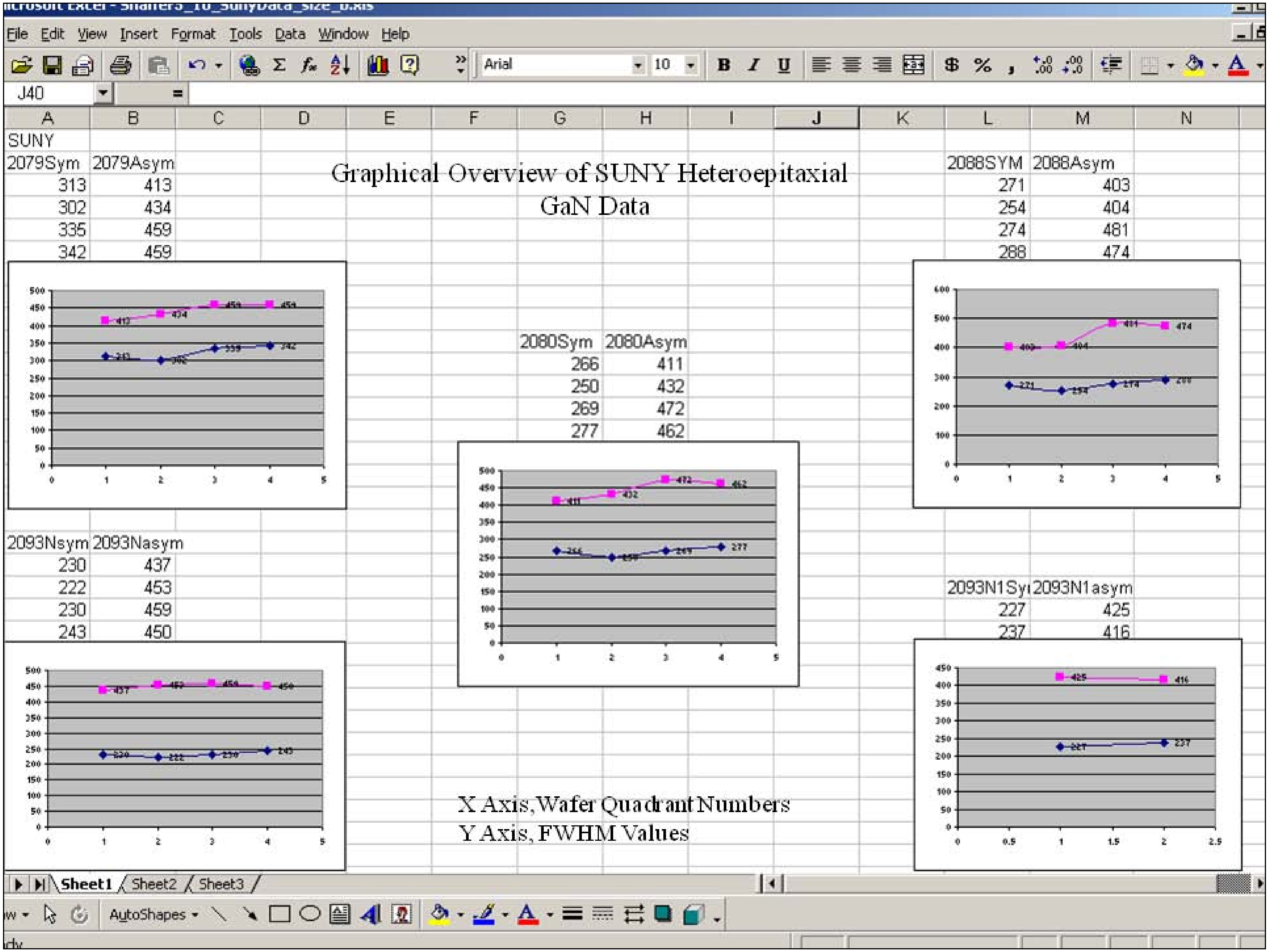



Figure 8. Graphical overview of SUNY heteroepitaxial GaN data. The sym scans are blue and the asym scans are red.

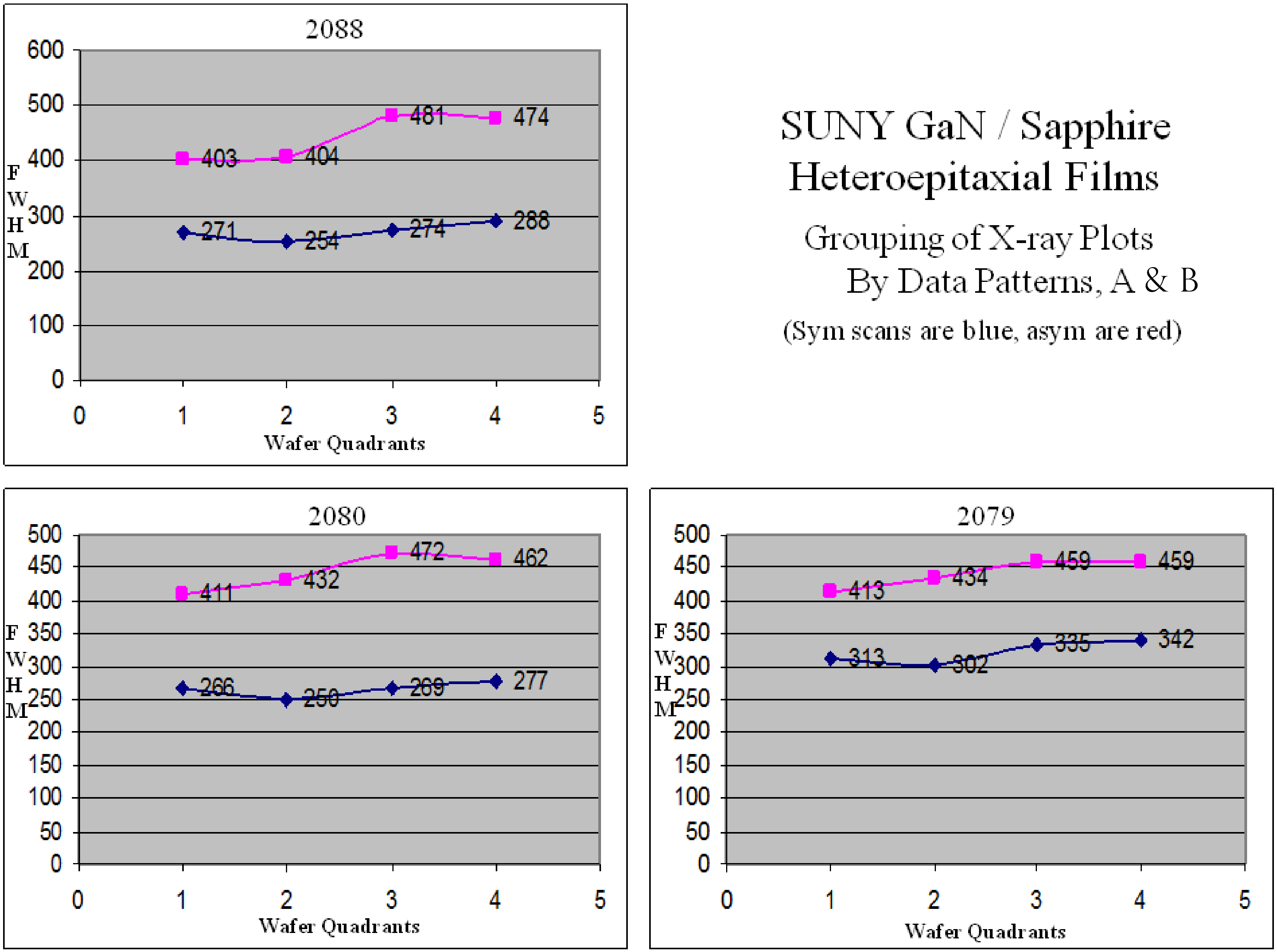
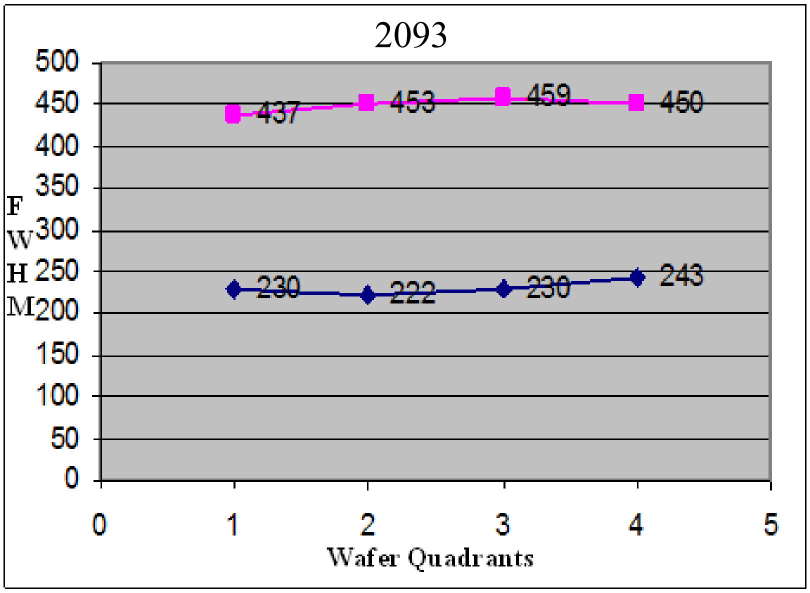



Figure 9. SUNY GaN/sapphire heteroepitaxial films, showing grouping of x-ray plots by data pattern A. The sym scans are blue and the asym scans are red.



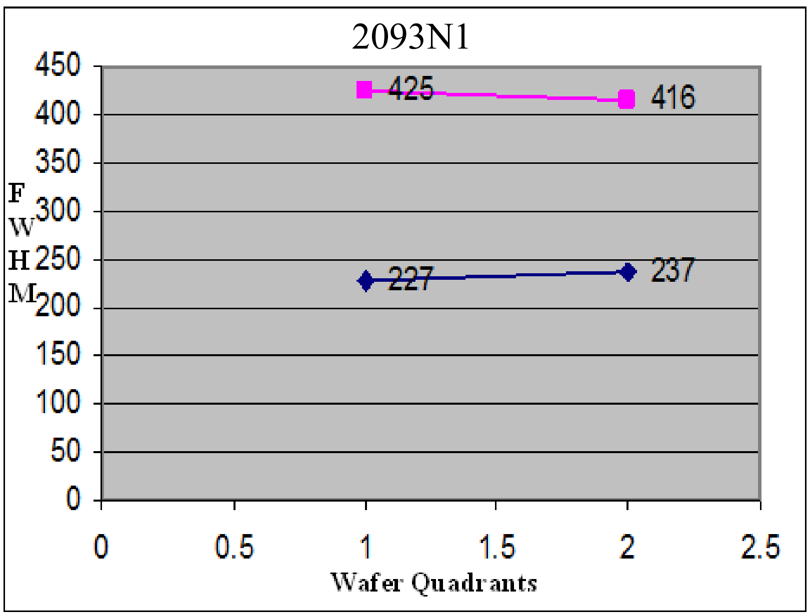




Figure 10. SUNY GaN/sapphire heteroepitaxial films, showing grouping of x-ray plots by data pattern B. The sym scans are blue and the asym scans are red.

## 4. GaN Substrates vs. GaN Films Grown On Them

This section presents a comparison of the structural quality of HVPE-grown GaN substrates and the metalorganic chemical vapor phase deposition (MOCVD) grown homoepitaxial GaN films produced on them. The data is represented in both table (table 1) and graphic (figure 11) forms. The following summary provides an additional examination of the data:

- The graphical output highlights the relationship between the substrates and films.
- The sym substrate and film scans track each other for both samples, but for the asym scans, they do not track for either sample.
- The sym values for both substrate and film of sample 8183 are excellent (table 1).
- The film values for the asym scans of 8184 contain an extraordinary value of 58”.
- The asym scans for the films are significantly lower than the substrate values, particularly for sample 8184.

These were the only homoepitaxial GaN films measured to date until a couple of weeks ago. Since then we have received a few samples from Lumilog/SUNY; however, they are not up to the level of quality of the Kyma samples examined here. The Lumilog/SUNY film’s sym values averaged ~200” and the film’s asym values averaged ~400”.

Table 1. GaN substrates vs. GaN films grown on them.

| **SAMPLE 8183** | **SAMPLE 8184** |
|---|---|
| **Sym Scan Values** | **Sym Scan Values** |
| Substrate: 49, 83, 65, 54<br>Film :50, 89, 66, 53 | Substrate: 74, 70, 132, 69<br>Film : 69, 62, 109, 59 |
| Notes | |
| Note: Very close match between substrate and film average values Sub 63”, Film 65” | Note: Similar average values, substrate and film: Sub 86”, Film 75”. |
| **Asym Scan Values** | **Asym Scan Values** |
| Substrate: 414, 484, 462, 402<br>Film : 268, 276, 291, 283 | Substrate: 477, 564, 670, 545<br>Film : 58, 106, 86, 71 |
| Notes | |
| Epi film numbers are 37% better than the substrate. Film 280” and Substrate 441”. | Substrate has values similar to 8183. Asym film values are very good, including a remarkable value of 58”. As a dataset, they are much better than the substrate’s asym values. |

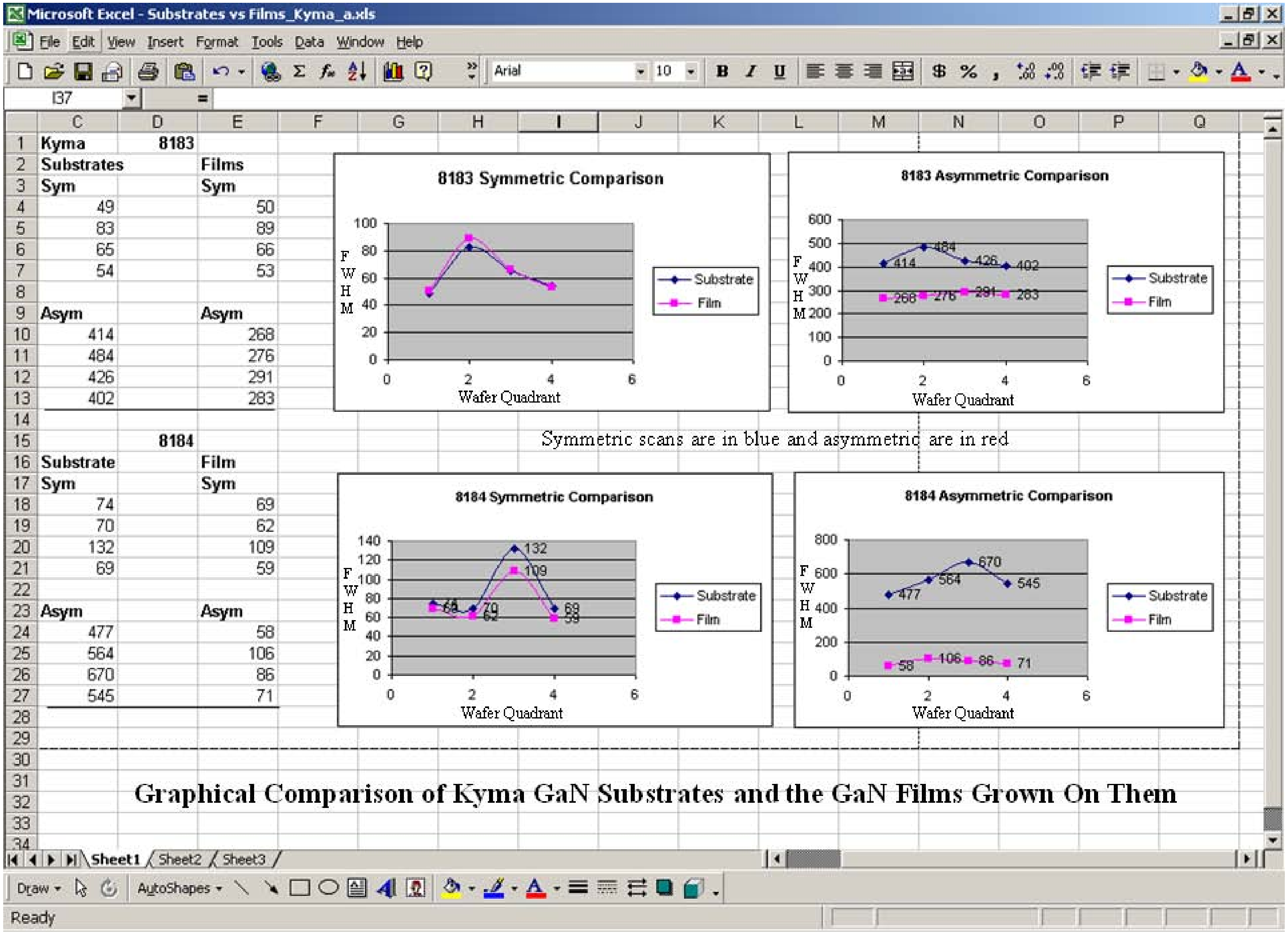



Figure 11. Graphical comparison of Kyma GaN Substrates and the GaN films grown on them, FWHM vs. quadrant plots

## 5. Homoepitaxial vs. Heteroepitaxial GaN Films

Two plots (sym and asym) containing eight scans were used to compare the homoepitaxial film data with the very good quality heteroepitaxial films we received, primarily, from our SUNY partners. Our team's principle grower, Mike Derenge, grew the homoepitaxial and heteroepitaxial films on the Kyma and the Crystal System's substrates, respectfully. All the SUNY and our principal grower's films were grown by MOCVD.

The comparisons for the sym scans show the homoepitaxial films improving over their heteroepitaxial counterparts by from 73% to 77% (figures 12 and 13). For the asym scans, the homoepitaxial films improved over their heteroepitaxial films by from 42% to 94%. It is very promising having two sym homoepitaxial FWHM values in the 50s, having an asym value in the 50s is extraordinary (i.e., sample 8184's 94% improvement). Good FWHM values correlate with lower defect densities, and lower defect densities are thought by the technical community to correlate with better device characteristics.

The homoepitaxial films show some remarkable improvements in crystal quality, unfortunately the devices that were fabricated on them had some performance issues. However, we do have initial data pointing to a solution for the device performance problems. Our group is currently in the process of implementing that solution.

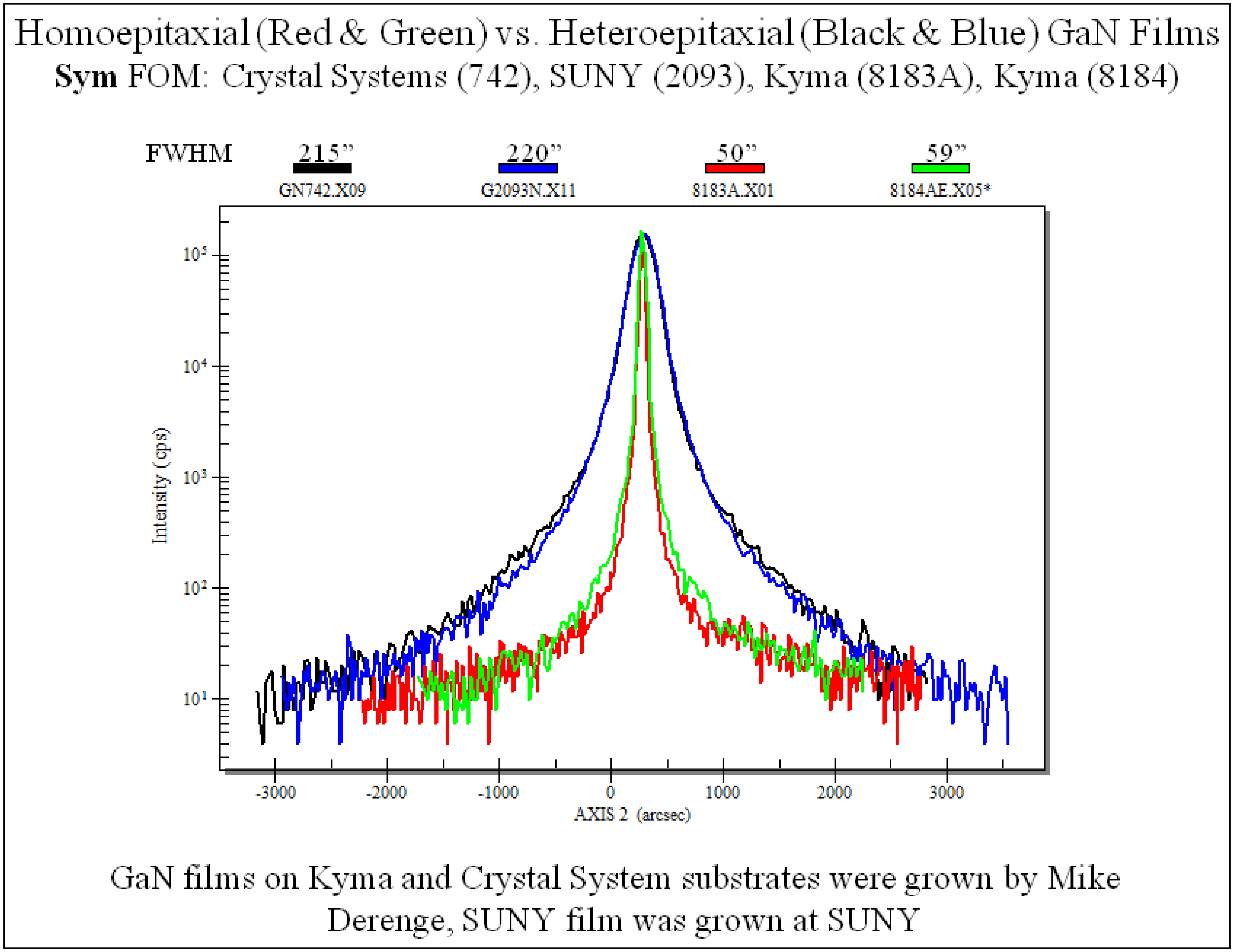



Figure 12. Comparison of homoepitaxial and heteroepitaxial films using sym scans.

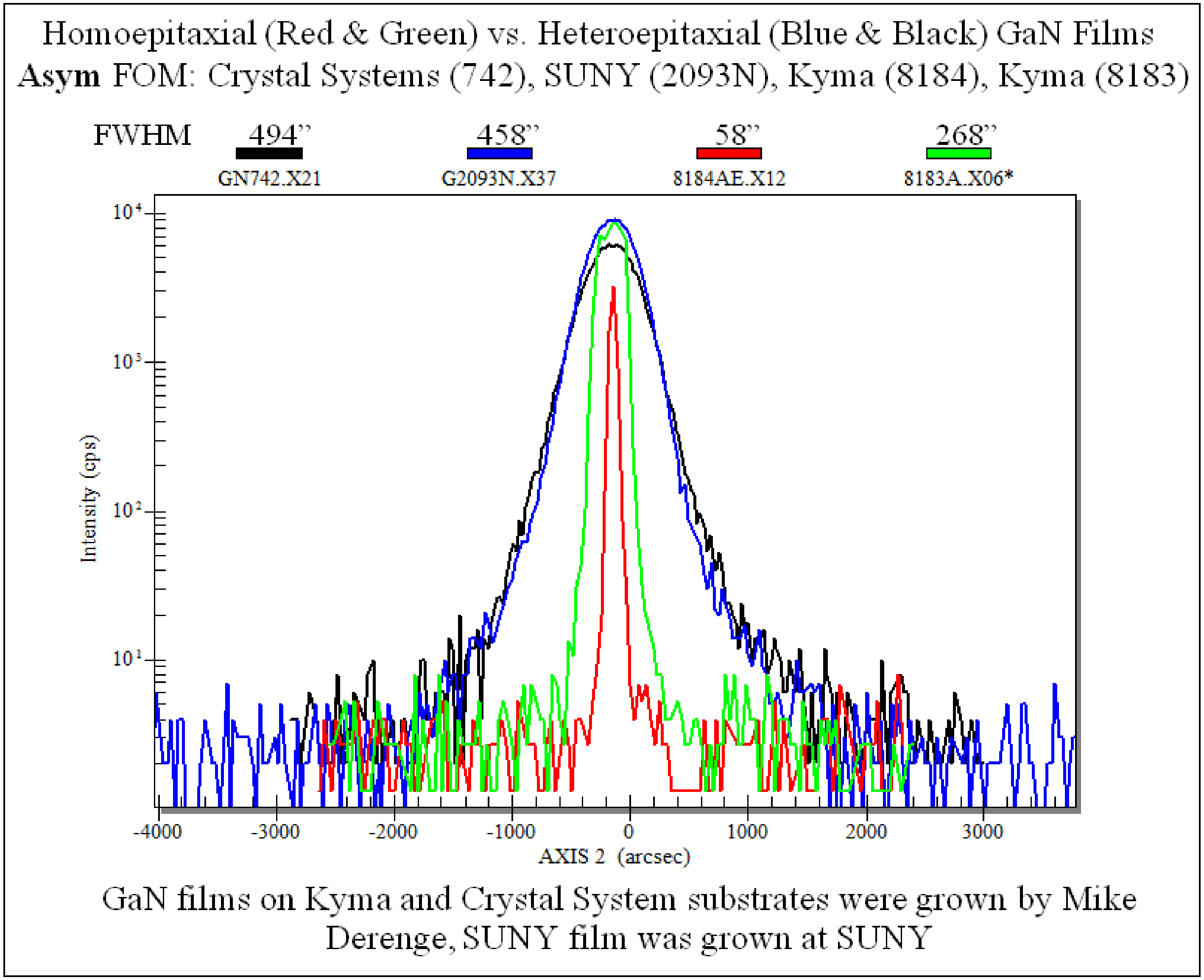



Figure 13. Comparison of homoepitaxial and heteroepitaxial films using asym scans.

# 6. Observations and Conclusions

In this interim report, I have presented the results of the microstructural analysis using x-ray diffraction of substrate and film inputs to the GaN WBG Device Program of the Power Components Branch.

We have observed the following:

- Our best GaN (002) FWHM value to date 39”. This is important because good FWHM numbers correlate with lower defect densities and lower defect densities are thought by the technical community to correlate with better device characteristics.
- We documented the quality of Kyma’s novel HVPE GaN substrates by wafer and wafer quarters (figures 1, 4, 5, and 6).
- We provided a composite thumbnail overview of the sample plots of Kyma’s novel GaN substrates (figure 3).
- We showed an example of the effect of peak broadening in x-ray output by SAGB (figure 2).
- Asym scans of 12 HVPE GaN substrate wafers show a broad range of FWHM values, ~350” to 1750” (figure 1).
- We had excellent asymmetric scan results of the homoepitaxial films (sample 8184) with FWHM values of 58” to 106” (table 1).
- We documented the good input quality of SUNY’s heteroepitaxial films by wafer and wafer quarters (figure 7).
- The composite thumbnail plots of SUNY scans provided an overview of heteroepitaxial film’s sym and asym scans to illustrate the relationships between them (figure 8).
- Homoepitaxial film quality showed improvement over the substrate it was grown on, in some cases by 5 to 7 times (Sample 8184, asym peaks, table 1).
- In sections 2, 3, and 4, we saw the variation in tracking between the sym and asym scans.
- We presented graphical comparisons between good quality GaN heteroepitaxial films and novel GaN homoepitaxial films from Kyma (figures 12 and 13).
- Kyma substrates’ micro-structural quality showed a bias across their 12 wafers in favor of quadrants I and IV (figure 1 and tables A-1 and A-2). This could be useful information for our Kyma partners.

There has been a steep learning curve in our team, and the technical community at large, regarding GaN quality. Recently, we have also obtained data suggesting we are overcoming a major hurdle involving carbon's negative role in the low-doped GaN films, which we use in fabricating some of our devices.

As we are able to obtain additional good homoepitaxial films to use for device fabrication, and our fabrication techniques and understanding matures, there will likely be additional useful and instructive correlations.

One group in the GaN device community has recently, after five years of hard work, achieved the technical community's target 600-V breakdown voltage. We have also attained 600-V breakdown on Kyma substrates and we are working to duplicate these results in our films.

While x-ray diffraction can help us rate our material input streams, it can also help inform us about issues like the material imperfections behind the material consistency issues we are working through. Going forward using x-ray diffraction along with scanning electron microscopy (SEM), Atomic Force Microscopy (AFM), cathodoluminescence (CL), and etch pit techniques, we will try to better understand and control the number and types of material defects in our devices to a degree that will help us have good device yields.

## Appendix. Statistical Bias between Kyma GaN Wafer Quadrants

The present data was examined to determine if the findings present in the report are statistically significant. Specifically, our goal was to determine if the mean FWHMs of the 002 (symmetric) reflections differed between quadrants of the Kyma samples. Two separate analyses were undertaken. First, the four quadrants were compared with the use of a two-factor analysis of variance (ANOVA). Second, the quadrants with the largest difference in mean, QI and QIII, were compared with a paired sample T-test.

The ANOVA analysis comparing the four quadrants is shown on table A-1. The 002 FWHM data are contained in the top table and are organized by wafer (row) and quadrant (column). Below the FWHM data is a tabulation of statistics on the individual columns (quadrants) which are used in the ANOVA calculation. For each column, the sum ($T_a$), sum squared ($T_a^2$), number of observations ($n_a$), mean, and standard deviation are calculated. Likewise, statistics are calculated by row (wafer) and tabulated to the right of the main data table. Below the table, the calculation steps are outlined, including calculation of the grand total $T$ and total number of observations $n$. Sum of squares variation due to factor A (that is, due to variation by column, or equivalently by quadrant of the wafer) $SS_A$ is calculated, along with the mean square variation due to factor A, $MS_A$. Likewise, the sum of squares and mean square variation $SS_B$ and $MS_B$ are calculated for variation due to factor B (that is, variation by row, or equivalently by wafer). The sum of squares due to interaction between the two factors $SS_{AB}$ is shown, along with the mean square variation $MS_{AB}$ (also known as error variance). Finally, the total sum of squares is given. Below these, the F value is given for variation due to factor A (data column or quadrant) and factor B (data row or wafer). The F value is given by $F_x = MS_x/MS_{AB}$, where $x$ is A or B. Next to the F value for both factors, the probability (from the F distribution) is given. The probability $P_A$ for factor A is interpreted as the probability that the four columns share the same mean. The value is 0.053, or equivalently there is a $1 - P_A = 0.947$ probability that the four columns (quadrants) do not have the same mean. Thus we have rigorously shown that there is a statistically significant difference in the mean value of the 002 FWHM depending on the quadrant of the wafer for these Kyma wafers.

Table A-1. Two factor ANOVA without replication.

## Two factor ANOVA without replication

| Wafer # | QI | QII | QIII | QIV | $T_b$ | $T_b^2$ | $n_b$ | Mean | Std. dev |
|---|---|---|---|---|---|---|---|---|---|
| **6921** | 82 | 84 | 173 | 114 | *453* | *205209* | *4* | *113.25* | *42.44* |
| **6942** | 56 | 61 | 54 | 54 | *225* | *50625* | *4* | *56.25* | *3.30* |
| **7041** | 56 | 69 | 93 | 82 | *300* | *90000* | *4* | *75.00* | *16.02* |
| **7286** | 76 | 119 | 130 | 69 | *394* | *155236* | *4* | *98.50* | *30.49* |
| **8183** | 49 | 83 | 65 | 54 | *251* | *63001* | *4* | *62.75* | *15.06* |
| **8184** | 74 | 70 | 132 | 69 | *345* | *119025* | *4* | *86.25* | *30.58* |
| **8185** | 167 | 154 | 157 | 154 | *632* | *399424* | *4* | *158.00* | *6.16* |
| **8186** | 58 | 60 | 66 | 57 | *241* | *58081* | *4* | *60.25* | *4.03* |
| **8187** | 72 | 157 | 85 | 72 | *386* | *148996* | *4* | *96.50* | *40.80* |
| **12932** | 100 | 101 | 104 | 120 | *425* | *180625* | *4* | *106.25* | *9.32* |
| **15691** | 39 | 39 | 40 | 41 | *159* | *25281* | *4* | *39.75* | *0.96* |
| **15994** | 54 | 60 | 61 | 65 | *240* | *57600* | *4* | *60.00* | *4.55* |

| | QI | QII | QIII | QIV |
|---|---|---|---|---|
| **$T_a$** | *883* | *1057* | *1160* | *951* |
| **$T_a^2$** | *779689* | *1117249* | *1345600* | *904401* |
| **$n_a$** | *12* | *12* | *12* | *12* |
| **Mean** | *73.583* | *88.083* | *96.667* | *79.250* |
| **Std. dev** | *33.776* | *37.744* | *42.934* | *33.251* |

| | | |
|---|---|---|
| **T** | 4051 | *Grand total* |
| **n** | 48 | *Total number of observations* |
| **$SS_A$** | 3690.7 | Sum of squares variation due to factor A (by column) |
| **$MS_A$** | 1230.2 | Mean square variation due to factor A (by column) |
| **$SS_B$** | 46388.2 | Sum of squares variation due to factor B (by row) |
| **$MS_B$** | 4217.1 | Mean square variation due to factor B (by column) |
| **$SS_{AB}$** | 14270.5 | Interaction sum of squares |
| **$MS_{AB}$** | 432.4 | Interaction mean square variation (also called error variance) |
| **$SS_{total}$** | 64349.5 | Total sum of squares |

| | F | P |
|---|---|---|
| **A (column)** | 2.845 | **0.053** |
| **B (row)** | 9.752 | 1E-07 |

*P is the probability that the different columns share the same mean*

| | | |
|---|---|---|
| F | 2.845 | *F statistic for variation between columns (quadrants)* |
| P | 0.053 | *Probability that different quadrants have same mean* |
| **P** | **0.947** | *Probability that different quadrants are statistically different (ie they do not have the same mean)* |

Table A-2 shows the T-test analysis. The two quadrants were chosen because they have the largest difference in mean value, 73.58 (QI) compared with 96.67 (QIII). The table shows the 002 FWHMs organized by wafer (row) and quadrant (column). To the right of the FWHM data, the mean for each row is given, as well as the difference *d* between the QI and QIII values for

each wafer. Below the table, statistics are calculated for each column (quadrant), including the mean, standard deviation, variance, and total number of observations $n$. The test statistic $t$ is given by

$$t = \frac{d_{avg}}{s_d / \sqrt{n}} \tag{A.1}$$

where $d_{avg}$ is the average difference between QI and QIII, $s_d$ is the standard deviation of the difference, and $n$ is the number of observations. From the test statistic, the t-distribution yields a probability of 0.024 that the two samples (quadrants I and III) have the same mean, that is, there is a 97.6% chance that they come from populations with different means. Thus, we can rigorously conclude that there is a significant difference in the means of the 002 FWHMs for quadrants I and III in the Kyma-grown GaN samples. Furthermore, from the $t$ value corresponding to a probability of 0.05, the 95% confidence interval for the mean difference between QI and QIII is found to be 19.34. Thus, we can say at a 95% confidence level that the difference between the mean values of QI and QIII is 23.08 ± 19.34. Further testing should help to narrow down the confidence window allowing us to more precisely determine the mean difference between the 002 FWHM of QI and QIII.

Table A-2. Paired sample T- test for QI and QIII.

**Paired sample T-test for QI and QIII**

| Wafer # | QI* | QII | QIII | QIV | Mean | d (QI - QIII) |
|---|---|---|---|---|---|---|
| 6921 | 82 | 84 | 173 | 114 | 113.25 | -91 |
| 6942 | 56 | 61 | 54 | 54 | 56.25 | 2 |
| 7041 | 56 | 69 | 93 | 82 | 75.00 | -37 |
| 7286 | 76 | 119 | 130 | 69 | 98.50 | -54 |
| 8183 | 49 | 83 | 65 | 54 | 62.75 | -16 |
| 8184 | 74 | 70 | 132 | 69 | 86.25 | -58 |
| 8185 | 167 | 154 | 157 | 154 | 158.00 | 10 |
| 8186 | 58 | 60 | 66 | 57 | 60.25 | -8 |
| 8187 | 72 | 157 | 85 | 72 | 96.50 | -13 |
| 12932 | 100 | 101 | 104 | 120 | 106.25 | -4 |
| 15691 | 39 | 39 | 40 | 41 | 39.75 | -1 |
| 15994 | 54 | 60 | 61 | 65 | 60.00 | -7 |
| **Mean:** | 73.583 | 88.083 | 96.667 | 79.250 | | -23.083 |
| **Standard dev:** | 33.776 | 37.744 | 42.934 | 33.251 | | 30.444 |
| **Variance:** | 1140.811 | 1424.629 | 1843.333 | 1105.659 | | 926.81 |
| **n:** | 12 | 12 | 12 | 12 | | 12 |

**Paired test, two tailed**

| | |
|---|---|
| -2.627 | Test statistic |
| 0.024 | Probability the two samples have the same mean |
| 0.976 | Probability the two samples do not have the same mean |
| **Mean difference:** | -23.083 |
| **95% confidence interval:** | 19.343 |

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## List of Symbols, Abbreviations, and Acronyms

| | |
|---|---|
| ANOVA | analysis of variance |
| Asym | asymmetric x-ray scan |
| CL | cathodoluminescence |
| FOM | figure of merit |
| FWHM | full width at half maximum |
| GaN | gallium nitride |
| HEMT | high electron mobility transistors |
| HVPE | hydride vapor phase epitaxy |
| MOCVD | metalorganic chemical vapor phase deposition |
| SAGB | small angle grain boundary |
| SEM | scanning electron microscopy |
| SUNY | State University of NY |
| Sym | symmetric x-ray scan |
| WBG | wide bandgap |

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